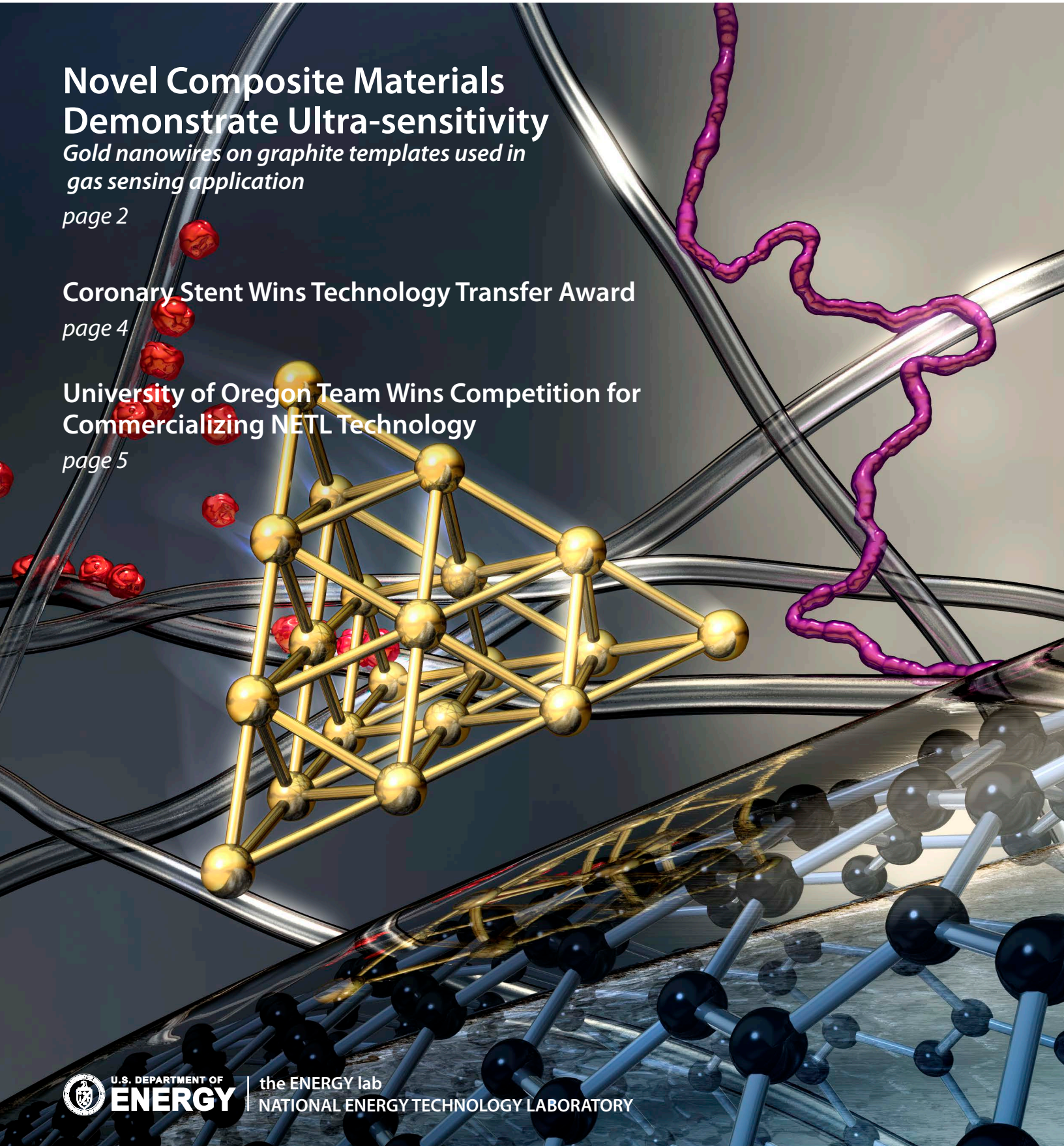
netlognews

NETL's R&D newsletter *April 2012, Issue 25*



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U.S. DEPARTMENT OF ENERGY | the ENERGY lab
NATIONAL ENERGY TECHNOLOGY LABORATORY

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Cover image: An artistic representation of the synthesis process of gold nanowires on functionalized single-walled carbon nanotubes. The growth mechanism of gold nanowires identified contains an ensemble of adsorption/desorption, shuttling and nanowelding elementary steps.

netlognews

newlognews is a quarterly newsletter that highlights recent achievements and ongoing research at NETL. Any comments or suggestions, please contact Paula Turner at paula.turner@netl.doe.gov or call 541-967-5966.

Novel Composite Materials Demonstrate Ultra-sensitivity

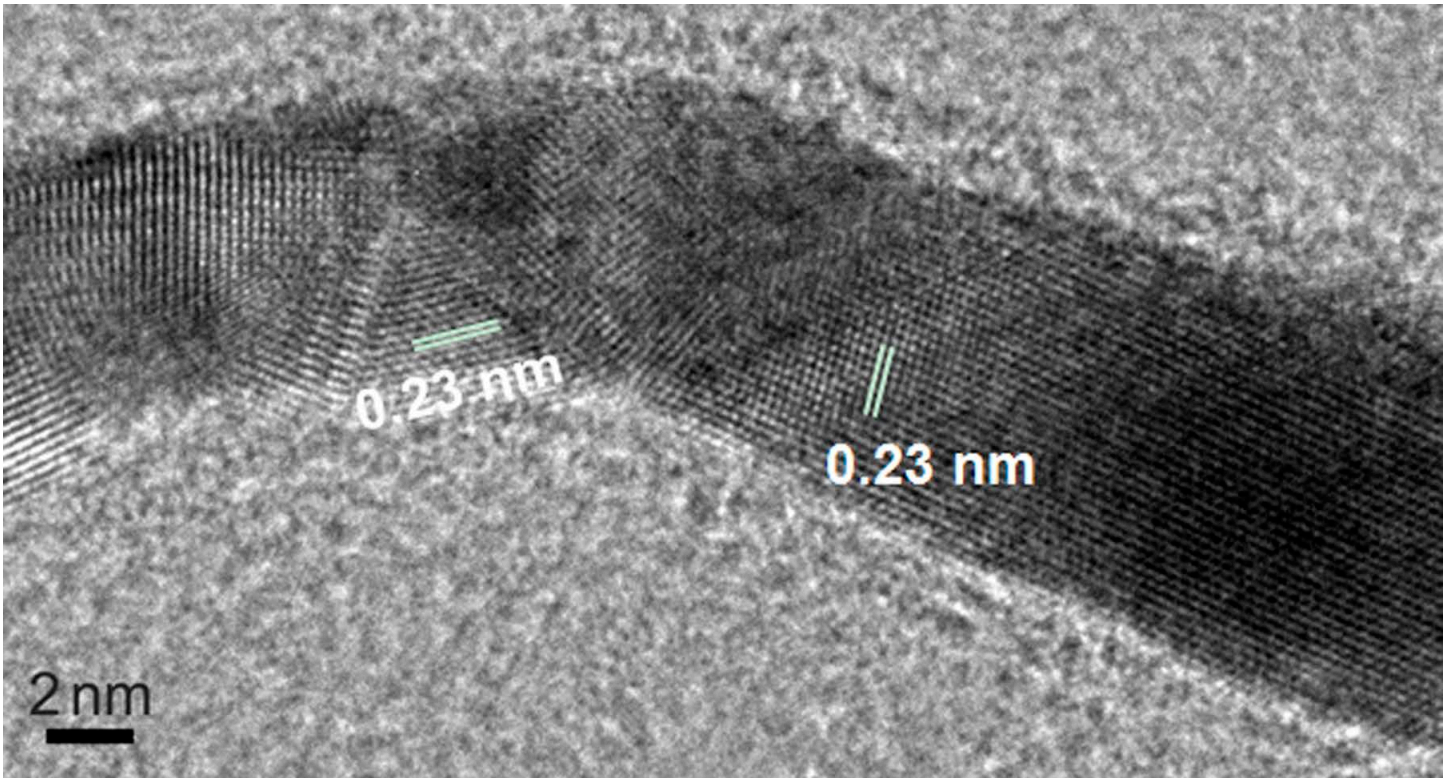
Gold nanowires on graphite templates used in gas sensing applications—Nanoscale building blocks allow scientists to create new complex architectures. The resulting novel materials have unique structures and functions that can achieve amazing laboratory results.

Scientists at the University of Pittsburgh and the National Energy Technology Laboratory (NETL) have successfully developed a method to self-assemble gold into nanowires for gas sensing applications. Their strategy is a bottom-up approach in which gold nanowires are built from gold nanoparticles in aqueous suspensions of single-walled carbon nanotubes treated with various coatings. In a complementary effort, the mechanisms that describe the observed growth of the gold nanowires, (composed of an ensemble of adsorption/desorption, shuttling and nanowelding) have also been deduced. The elementary steps of this mechanism were demonstrated through first principles density functional theory calculations and validated with X-ray diffraction and transmission electron microscopy measurements.

In tests to determine the composite materials' effectiveness in sensing applications, an ultra-sensitivity to hydrogen sulfide in both the parts per billion (ppb) and parts per million (ppm) concentrations was demonstrated with a detection limit as low as 5 ppb at room temperature. A hybrid gold nanowire-carbon nanotube material, and the associated device, has potential application as a portable detection sensor in very diverse areas ranging from the natural gas industry to personal safety and personal healthcare.

The results of this combined experimental and theoretical study were recently published in the premier *Journal of the American Chemical Society:* "Welding of Gold Nanoparticles on Graphitic Templates for Chemical Sensing" by Mengning Ding, Dan C. Sorescu, Gregg P. Kotchey, and Alexander Star.

The importance of the results obtained resides not only in development of a synthesis method to grow gold-nanowires on carbon nanotubes templates, but in



High-resolution transmission electron microscope image of gold nanowires showing the polycrystalline nature of the welded gold nanowires. Image courtesy of the University of Pittsburgh.

a development, based on both experimental and first principles computational results, of a nanowelding model that explains the overall growth mechanism. Additionally, the composite materials obtained were tested for gas sensing applications and an ultra-sensitivity to hydrogen sulfide to levels as low as 5 parts per billion was demonstrated. The nanowelding of the gold nanowires results was characterized in a *C&EN News* article by Reginald Penner, a chemist at the University of California, Irvine as "strikingly original."

Development of chip-based sensors that rely on nanomaterials to detect hydrogen sulfide in complex mixtures of gases also opens practical ways to create portable and less expensive devices with direct applications in natural gas and gas well industries, personal safety and healthcare. Carbon nanotubes are one of the most promising inorganic templates for this strategy because of their unique physical, chemical, and mechanical properties, which translate into numerous potential applications.

A *CE&N News* story written by Katherine Bourzac about this technology, "Gold Nanowires Sense Gas," can be found here.

Contact: Dan Sorescu, 412-386-4827

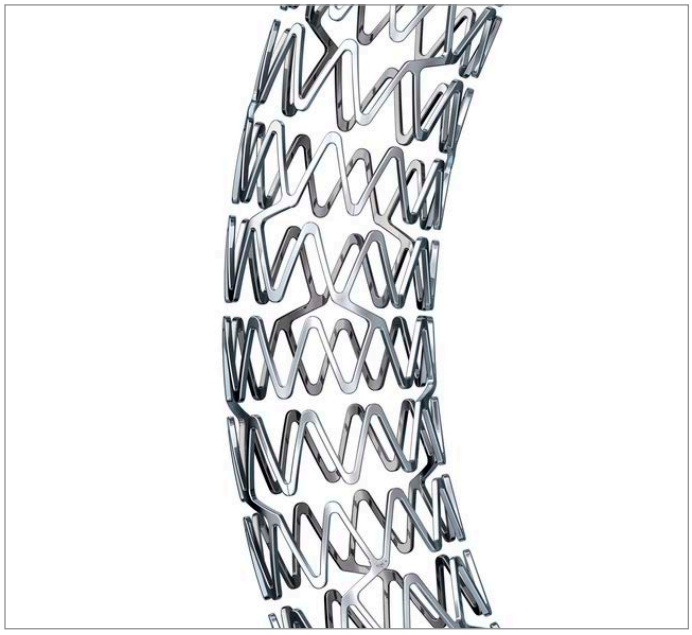
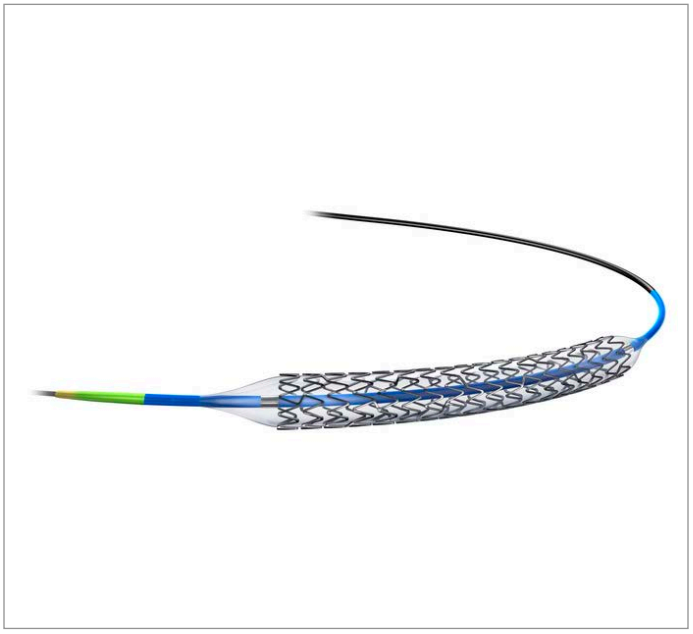


Illustration of the award-winning stent structure, courtesy of Boston Scientific.



PROMUS Element™ Plus Platinum Chromium Everolimus-Eluting Stent System – showing catheter delivery system. Image courtesy of Boston Scientific.

Coronary Stent Wins Technology Transfer Award

—A new coronary stent, which incorporates an innovative metal alloy developed by scientists at Boston Scientific Corporation, Inc. (BSCI) and NETL, has been selected to receive a 2012 Award for Excellence in Technology Transfer. BSCI, the commercialization partner, utilized the improved alloy performance to develop new coronary stent products with superior properties compared with existing stainless steel stents.

Global sales since market entry are now approaching $3 billion, representing a 45 percent share of the coronary stent market. BSCI has announced that all future stents will utilize this innovative alloy in its manufacture. Sales are expected to further increase as cardiovascular surgeons learn more about the unique features and patient benefits using these innovative coronary stents.

This national award is presented annually by the Federal Laboratory Consortium for Technology Transfer (FLC) in recognition of outstanding work by researchers in the transfer of technology from federal laboratories to the commercial marketplace. NETL's Paul Turner, Paul Jablonski, and Edward Argetsinger will receive the award for their effort on this collaborative project. Award applications were reviewed by a panel of technology transfer experts representing industry, state and local government, academia, and the federal laboratory system.

The FLC is a nationwide network of federal laboratories that promotes the rapid transfer of laboratory research results and technologies into the marketplace. Its national and regional awards programs recognize laboratory employees who have done outstanding work in technology transfer over the past year. NETL is one of more than 250 federal laboratories and centers, along with their parent departments and agencies that are members of the FLC.

In related news, Boston Scientific has announced the European market launch of the PROMUS Element™ Plus platinum chromium coronary stent. The stent also incorporates the NETL/BSCI-developed platinum chromium (PtCr) alloy. Boston Scientific states in its announcement that "The PtCr alloy and stent architecture used in the Element platform offer significant advantages in conformability and radiopacity compared to other stent platforms."

Recently, an Italian doctor implanted the first patient in Europe with the device and stated, "I believe the improved deliverability of the PROMUS Element Plus Stent System will add another significant benefit, especially when accessing challenging lesions. This innovative stent is also supported by strong clinical outcomes from the PLATINUM trials, which demonstrated very low rates of revascularization and stent thrombosis at one year."

Boston Scientific believes that this new product line will increase their coronary stent market share dramatically. Boston Scientific plans to immediately market the stent in select European and other CE Mark* countries. It also has been recently approved by the FDA for sale in the United States.

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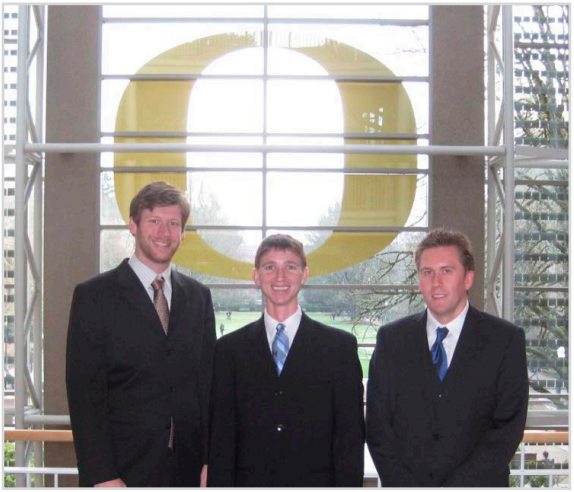
*The CE Mark on a product or machine identifies it as complying with all the of safety requirements established by the European Union.



Corrosion Solutions team *from the University of Oregon.*

University of Oregon Team Wins Competition for Commercializing NETL Technology

—A team of students at the University of Oregon is working to develop commercial opportunities for NETL's patented Cerium Surface Treatment. Like any small startup company, they needed a name and chose *Corrosion Solutions*. In the fall quarter, *Corrosion Solutions* wrote a business plan and presented it to a panel of reviewers.

The plan was very well received and the team was invited to participate in the University of Oregon's Venture Capital Start-Up class.

The Cerium Surface Treatment technology is a chemical surface modification that protects stainless steel from heat-induced corrosion and thus increases a product's useful life. The *Corrosion Solutions* team is finalizing a license with NETL to use this technology to market a number of products for home and industrial applications.

This team participated in the Mai Business Plan Competition in Bangkok, Thailand, March 1-3 and was awarded first place – the *H.M. The King of Thailand Award* – in the competition, as well as awards for *Best Presentation and Most Professional* during the opening rounds of the competition.

The field of competitors comprised 55 teams from 23 countries, representing 6 continents. The first place win came with a $12,000 cash award along with admittance to the Bangkok Executive Entrepreneur Training Center (a $14,000 value). The team also received entry to the MIT-sponsored International Investment Competition in Istanbul in March. Further details about the Thailand award can be found at: www.bbc.in.th.

NETL scientist Dr. Paul Jablonski, co-inventor of the Cerium Surface Treatment, will continue to advise the team.

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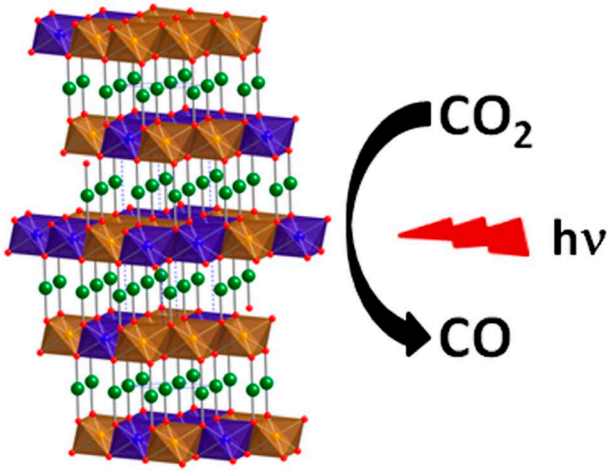


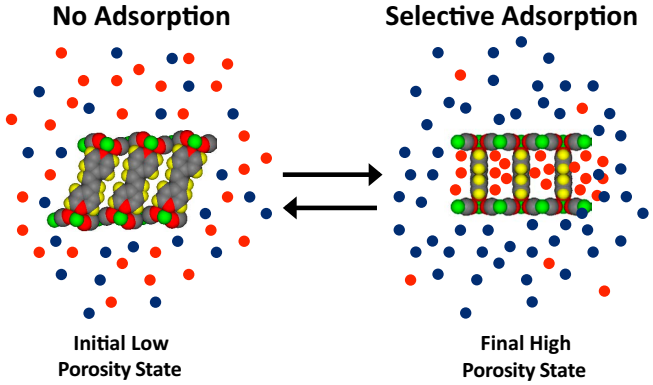
Delafossite materials use light to reduce CO_2 to CO.

NETL, WVU Researchers Design New Catalysts for CO_2 Management

—The photocatalytic reduction of carbon dioxide to C1 products such as carbon monoxide, methane, and methanol has the potential to simultaneously reduce CO_2 emissions and create an industrial product stream, which could be sold to offset the costs associated with the deployment of carbon capture and sequestration technologies. Current challenges associated with photocatalysts for this process include low optical activity in the visible region of the solar spectrum, slow reaction kinetics, and poor product selectivity due to band alignment mismatches. Due to unique physical properties, delafossite materials have the potential to address several of these issues, making them attractive candidates for CO_2 management applications.

Researchers at NETL and West Virgina University have used a combination of computational and experimental methodologies to show that iron substitution in $CuGaO_2$ delafossites can control the optical activity of this material by creating new electronic states in the material. Iron substitution was successful in modifying $CuGaO_2$ from a material which only absorbed high-energy ultraviolet light to one capable of absorbing a broad range of light frequencies from the low-energy near infrared up to the high-energy ultraviolet region. The research illustrates the potential of delafossites for a variety of optical and photocatalytic applications which require tunable optical properties. The research team recently published the results in the prestigious *Journal of Physical Chemistry C* (Vol. 116, 2012, p. 1865-1872)

Contact: Jonathan W. Lekse, 412-386-7312



Schematic illustration showing the opening of a structurally dynamic MOF sorbent with selective adsorption of one gas over another. CO_2 (represented in red) can both open and energetically stabilize the high porosity state of the MOF. Experiments show other gases, such as N_2 and CH_4 (represented in blue) cannot, thus leading to the selective adsorption observed by NETL researchers.

Structurally Dynamic MOF Sorbent Selectively Adsorbs CO_2 from Gas Mixtures

—Gas separations are important to many areas of fossil energy including pre- and post-combustion CO_2 capture, as well as fuel cell applications. The need for efficient gas purification processes has led to interest in developing a new class of sorbents at NETL that can successfully separate carbon dioxide from mixtures of light gases such as methane and nitrogen, thus paving the way for more extensive testing of these materials.

The sorbents are based on a structurally dynamic metal-organic framework (MOF) material called "NiDBM" which selectively transitions from a low to high porosity state in the presence of CO_2. Since CO_2 is responsible for initiating the structure change as well as for stabilizing the high porosity state, other gases in the mixture are not adsorbed within the pore-network of the sorbent.

The sorbent's selectivity was evaluated in situ using infrared spectroscopy, neutron diffraction techniques, and gas chromatography in order to probe the structure and gas mixture changes associated with selective adsorption. The results from this work were recently published in the high-impact factor journal, *Angewandte Chemie International Edition* (Vol. 50, pgs 10888-10892).

Contact: Christopher Matranga, 412-386-4114

Scientist using Engineering-Process Simulator Interface.

Award-winning NETL Software Successfully Interfaced with Chemical Process Simulator—

Collaborators at NETL and Ames Laboratory have integrated the open-source chemical process simulator DWSIM with their R&D 100 award-winning Virtual Engineering-Process Simulator Interface (VE-PSI). Integrating an open-source process simulator with VE-PSI creates a unique rapid design environment in which virtual prototypes for new plant designs can be quickly created and easily reviewed. Design of next-generation energy plants that reduce environmental impacts in a cost-effective manner requires collaboration between a broad range of shareholders including engineers, scientists, operators, and owners. The immersive, interactive, and three-dimensional, plant walk-through created by VE-PSI enables these stakeholders to view, update, and design a virtually operating plant.

The project team also verified the ability of VE-PSI to work with industry-accepted compliant flow sheets and interface with dynamic data from Invensys™ DYNSIM, an Invensys™ product for designing and operating a modern process plant safely and profitably. With these latest features VE-PSI supports these simulators: Aspen Plus®, Aspen Plus Dynamics®, Invensys™ DYNSIM, MathWorks® Simulink®, Powersim, and DWSIM.

Creating an integrated research, design, and training environment allows energy plant operators to gain an improved understanding of an advanced power generation facility before actually stepping foot in a real plant. This will reduce the cost and time needed to go from an advanced energy plant concept to a clean, low impact energy plant.

Contact: Steven M. Seachman, 304-285-5448

Gasifier Modeling Software Available for Use with NETL Co-Simulator Software—

As part of an NETL Advanced Research project, Reaction Design, a software and services provider, has extended its ENERGICO software to automatically and systematically generate multi-zonal gasifier models. ENERGICO is a simulation tool for designing clean combustion systems in gas turbines and burner applications. The multi-zonal models are a category of reduced order models (ROMs) that approximate high-fidelity computational fluid dynamics (CFD) simulations of multiphase-flow gasifiers—the centerpiece of integrated gasification combined cycle power plants. The CFD-based multi-zonal ROMs are implemented as an equivalent reactor network (ERN) in Reaction Design's CHEMKIN-PRO, a combustion chemistry simulation software.

The ERN's are compliant with the process industry CAPE-OPEN (CO) software standard, enabling them to be used with NETL's CO-compliant Advanced Process Engineering Co-Simulator (APECS).

This combination enables process and energy companies to achieve their clean technology goals by automating the analysis of processes via computer simulation and modeling solutions.

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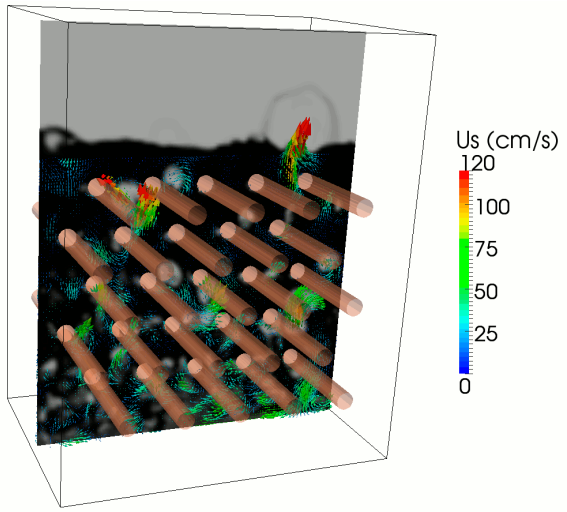


Click Here for MFIX video

MFIX simulation of a fluidized bed with submerged tube bundle.

Researchers Announce Latest Version Release of MFIX

—The latest release of NETL's multiphase computational fluid dynamics (CFD) solver MFIX is available for download at https://mfix.netl.doe.gov. MFIX is a general purpose computer code developed by NETL for describing the hydrodynamics, heat transfer, and chemical reactions in fluid-solids systems. The MFIX solvers (MFIX-continuum and the latest Lagrangian particle tracking solver MFIX Discrete Element Model or MFIX-DEM) are both open source software.

The new parallelization strategy in the latest MFIX release now allows simulations of upwards of 10 million particles with MFIX-DEM. The addition of heat and mass transfer in MFIX-DEM allows a user to simulate reacting particle flows for a variety of fossil fuel devices with carbon management. The MFIX-DEM solver also paves the way for developing hybrid solvers (continuum and Lagrangian) to address the need for fidelity without additional computational costs. Moreover, the improvement to the cut-cell grid technology enables the use of more complex geometry in MFIX.

In an effort to characterize the uncertainty associated with computer simulation of multiphase flows, MFIX has been interfaced with open source uncertainty quantification (UQ) toolbox software PSUADE (Problem Solving environment for Uncertainty Analysis and Design Exploration) from the Center for Applied Scientific Computing (CASC) of the Lawrence Livermore National Laboratory. This new capability enables MFIX users to perform various UQ related analysis, which was not available previously.

This capability now allows a user to:

- create and run statistically-designed simulation experiments to extract maximum information with a minimum number of runs,
- do a sensitivity study to better understand the relationship between set input variables and output, and
- forward propagation of input uncertainties to estimate output uncertainty and Markov Chain Monte Carlo (MCMC) approach-based Bayesian model calibration to utilize experimental data with simulation data for systemic calibration of model parameters.

The new capability is a critical addition to the portfolio of analysis tools available for future UQ activities at NETL.

MFIX has a user base that includes over 2600 registrants in over 70 countries. The next major release of MFIX is scheduled for the end of 2012.

Contact: Mehrdad Shahnam, 304-285-4546

Helicopters equipped with two boom-mounted cesium magnetometers have been used by NETL to locate wells in Wyoming.

NETL Uses Helicopter Magnetic Surveys to Locate Abandoned Oil and Gas Wells in Pennsylvania

—On March 9-12, 2012, NETL contracted an aeromagnetic survey over an area of Washington County, Pennsylvania, where past oil and gas production had occurred and where future Marcellus Shale gas production is expected. The survey's purpose was to locate existing wells based on the unique perturbation of the earth's magnetic field caused by vertical steel well casing.

The helicopter-based Fugro Midas II™ system used for the survey employs twin cesium ion vapor magnetometer sensors that are boom-mounted 12.5 m apart and oriented orthogonally to the flight path. The 290 line kilometer, 735 hectare survey was designed to optimize the detection of ferromagnetic targets that are susceptible to Earth-induced magnetization such as steel well casings. A close, nominal line spacing of 25 m afforded generous overlap and excellent aerial coverage improving the likelihood that all significant magnetic anomalies would be detected. An altitude of 30 m was selected to reduce potential terrain conflicts and maximize sensitivity.

A proprietary hardware and software system compensates for the unwanted magnetic aberrations caused by the maneuvering of the helicopter, electronic interference, and eddy currents. Preliminary results indicate that the survey correctly located known wells and identified numerous other magnetic anomalies that are likely to be wells. A ground investigation is underway to identify the ferromagnetic source for magnetic anomalies believed to be unknown wells.

Contact: Garret Veloski, 412-386-5809

Palladium Sorbents Show Extraordinary Capabilities

—In August, 2011, Southern Company tested a 10 pound bed of a 2 weight percent palladium on alumina sorbent beads in a slipstream of PRB coal-derived sour fuel gas at its Wilsonville, Alabama Pilot Facility. The sorbent was exposed to the syngas for 1011 hours (over 42 days) at 500˚ F, a pressure of 180 psig, and a space velocity of 1704 hours. The syngas entering and exiting the sorbent reactor was periodically monitored for mercury, arsenic and selenium by modified versions of EPA Methods 29 and 30. The used sorbent was also analyzed for mercury and other elements.

Palladium sorbents developed at NETL have been found to effectively capture trace contaminants such as mercury, arsenic, selenium, and phosphorus at elevated temperatures from syngas. Johnson Matthey licensed the technology from NETL in 2007 for application to coal gasification plants and is currently testing the technology at larger scales. The technology received the R&D 100 award in October 2008. While many sorbents have been demonstrated for near-ambient temperature removal of mercury from natural gas and syngas, and for removal of mercury from flue gas at temperatures up to 350˚F, few sorbents have been shown to remove mercury, arsenic and selenium from high temperature syngas.

The NETL sorbent removed nearly 100 percent of the mercury present within the syngas, with no breakthrough observed. This was the fifth and more challenging long-term exposure of the palladium to slipstreams of syngas at this pilot facility; and Johnson Matthey is planning a sixth long-term test for 2012. In each of the previous tests the sorbent removed nearly all of the trace contaminants. These are outstanding results for multi-pollutant control of the trace elements.

The sorbents are described in US patent 7,033,419, issued in April 2006, and in recent issues of the journals *Industrial & Engineering Chemistry Research, Fuel, and Main Group Chemistry*.

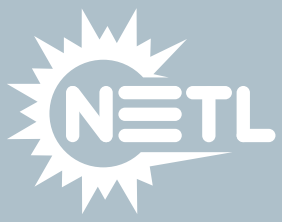
Contact: Evan J. Granite, 412-386-4607 and Henry W. Pennline, 412-386-6013

Recent NETL Publications

1.	Jeongho, Kim; Massoudi, Mehrdad; Antaki, James F. et al. February 15, 2012. Removal of Malaria-Infected Red Blood Cells Using Magnetic Cell Separators: A Computational Study, *Applied Mathematics and Computation*, 218 (12) 6841-6850.
2.	Liu, Yong; Gamwo, Isaac K. February 2012. Comparison Between Equilibrium and Kinetic Models for Methane Hydrate Dissociation, *Chemical Engineering Science*, 69 (1) 193-200.
3.	Jones, Dustin; Bhattacharyya, D.; Turton, R.et al. February 2012. Rigorous Kinetic Modeling and Optimization Study of a Modified Claus Unit for an Integrated Gasification Combined Cycle (IGCC) Power Plant with CO_2 Capture, *Industrial and Engineering Chemistry Research*, 51 (5) 2362-2375.
4.	Massoudi, Mehrdad; Vaidya, Ashwin. February 2012. Analytical solutions to Stokes-type flows of inhomogeneous fluids Massoudi Mehrdad; Vaidya Ashwin *Applied Mathematics and Computation*, 218 (11) 6314-6329.
5.	Rupp, Erik C.; Granite, Evan J.; Stanko, Dennis C. February 2012. Catalytic Formation of Carbonyl Sulfide During Warm Gas Clean-up of Simulated Coal-Derived Fuel Gas with Pd/gamma-AI(2)O(3) Sorbents, Fuel, 92 (1) 211-215.
6.	Fang, H.Z., Wang; W.; Jablonski, Paul D. et al. January 30, 2012. Effects of Reactive Elements on the Structure and Diffusivity of Liquid Chromia: An Ab Initio Molecular Dynamics Study, *Physical Review B*, 85 (1) Article Number: 014207.
7.	Lekse, Jonathan W.; Underwood, M. Kylee; Lewis, James P. et al. January 19, 2012. Synthesis, Characterization, Electronic Structure, and Photocatalytic Behavior of CuGa02 and CuGal-xFex02 (x=0.05. 0.10. 0.15. 0.20) Delafossites, J. *Physical Chemistry C*, 116 (2) 1865-1872
8.	Shi, Wei; Myers, Christina R.; Luebke, David R.; et al. December 2011. Theoretical and Experimental Studies of CO_2 and H_2 Separation Using the 1-Ethyl-3-methylimidazolium Acetate ([emim][CH_3COO]) Ionic Liquid, J. *Physical Chemistry B*, 116 (1) 283-295.
9.	Mohaghegh, Shahab D.; Gruic, Ognjen; Zargari, Saeed; et al. 2012. Top-Down, Intelligent Reservoir Modelling of Oil and Gas Producing Shale Reservoirs: Case Studies, *Intl. J. Oil Gas & Coal Technology*, 5 (1) 3-28.
10.	Spivak-BimdorfLev, J.; Stewart, Brian W.; Capo, Rosemary C.; et al. January 2012. Strontium Isotope Study of Coal Utilization By-Products Interacting with Environmental Waters, *J. Environmental Quality*, 41 (1) 144-154.
11.	Priyadarshini, Deepika; Kondratyuk, Petro; Miller, James B.; et al. January 2012. Compact Tool for Deposition of Composition Spread Alloy Films, J. Vacuum *Science & Technology A*, 30 (1) Article Number: 011503.
12.	Phuoc, Tran X.; Chen, Ruey-Hung. January 2012. Modeling the Effect of Particle Size on the Activation Energy and Ignition Temperature of Metallic Nanoparticles, *Combustion and Flame*, 159 (1) 416-419.

Patents Issued This Quarter

1.	Oxy-fuel Combustion With Integrated Pollution Control; Thomas L. Ochs, Brian Patrick (Jupiter Oxygen Company), Cathy A. Summers, Danylo Oryshchyn, Paul C. Turner, Patent number **8,087,926**, issued January 3, 2012.
2.	Electric Current Locator; Paul E. King, Charles R. Woodside, Patent number **8,111,059**, issued February 7, 2012.
3.	Apparatus and Method for Determining Solids Circulation Rate, J. Christopher Ludlow, James Spenik, Patent number **8,116,992**, issued February 14, 2012.
4.	Process for CO2 Capture Using Zeolites from High Pressure and Moderate Temperature Gas Streams; Ranjani V. Siriwardane, Robert Stevens (Parsons), Patent number **8,128,735**, issued March 6, 2012.
5.	Pyrochlore-type Catalysts for the Reforming of Hydrocarbon Fuels; David A. Berry, Dushyant Shekhawat, Daniel Haynes (ORISE), James Jerry Spivey (ORISE; LSU), Mark Smith (URS), Patent number **8,133,463**, issued March 13, 2012.
6.	Methods of Reforming Hydrocarbon Fuels Using Hexaaluminate Catalysts; Todd H. Gardner, David A. Berry, Dushyant Shekhawat, Patent number **8,142,756**, issued March 27, 2012.



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